Research article

On leap Zagreb indices of bridge and chain graphs

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Abstract: The 2-degree of a vertex $v$ in a (molecular) graph $G$ is the number of vertices which are at distance two from $v$ in $G$. The first leap Zagreb index of a graph $G$ is the sum of squares of the 2-degree of all vertices in $G$ and the third leap Zagreb index of $G$ is the sum of product of the degree and 2-degree of every vertex $v$ in $G$. In this paper, we compute the first and third leap Zagreb indices of bridge and chain graphs. Also we apply these results to determine the first and third leap Zagreb indices of some chemical structures such as polyphenyl chains and spiro chains.

Keywords: leap Zagreb indices; bridge graphs; chain graph

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1. Introduction

A molecular graph in chemical graph theory is the graphical representation of the structural formula of a chemical compound in which the vertices represent atoms and edges represent chemical bond between those atoms. A topological index of a molecular graph $G$ is a real number which characterizes the topology of $G$. Also it is invariant under graph automorphism. Topological indices have been widely used in Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies. It has application in many folds, to name a few areas, biochemistry, nanotechnology, pharmacology. Bond energy is a measure of bond strength of a chemical compound. The distance between two atoms is considered as the bond length between them. The higher the bond energy, the smaller is the bond length between those atoms. The recently introduced 2-degree based topological invariants, analogous to novel graph invariants (Zagreb indices), namely leap Zagreb indices, may be applied in studying such bond energy between atoms in
a molecular graph of a chemical compound.

Throughout this paper, \( G = (V, E) \) represents a connected molecular graph with the vertex set \( V(G) \) and the edge set \( E(G) \). Let the number of vertices and edges of \( G \) be \( n \) and \( m \) respectively. The degree of a vertex \( v \) in \( G \) is the number of vertices adjacent to \( v \) in \( G \) and denoted by \( \text{deg}(v : G) \). The 2-degree (or the second-degree) of a vertex \( v \) in \( G \) is the number of vertices which are at distance two from \( v \) in \( G \) and denoted by \( d_2(v : G) \). The Zagreb indices, namely, the first and second Zagreb indices, are the most important and oldest molecular structure descriptors. These indices have been studied extensively in the field of Mathematical Chemistry [3–5]. Recently, the concept of Forgotten topological index also known as F-index have attracted many researchers which results in over 100 research articles related to F-index. A.M.Naji et al. [13] have recently introduced and studied some properties of a new topological invariant called Leap Zagreb indices. They are defined as follows:

\textbf{Definition 1.} (i) The first leap Zagreb index \( LM_1(G) \) of a graph \( G \) is equal to the sum of squares of the second degrees of the vertices, \( LM_1(G) = \sum_{u \in V(G)} d_2(u)^2 \).

(ii) The second leap Zagreb index \( LM_2(G) \) of a graph \( G \) is equal to the sum of the products of the second degrees of pairs of adjacent vertices, \( LM_2(G) = \sum_{uv \in E(G)} d_2(u)d_2(v) \).

(iii) The third leap Zagreb index \( LM_3(G) \) of a graph \( G \) is equal to the sum of the products of the degree with the second degree of every vertex in \( G \), \( LM_3(G) = \sum_{u \in V(G)} \text{deg}(u)d_2(u) \).


First, we recall the definitions of bridge and chain graphs from [1] as follows:

\textbf{Definition 2.} Let \( \{G_i\}_{i=1}^d \) be a set of finite pairwise disjoint graphs with distinct vertices \( v_i \in V(G_i) \). The bridge graph \( B_1 = B_1(G_1, G_2, \ldots, G_d; v_1, v_2, v_3, \ldots, v_d) \) of \( \{G_i\}_{i=1}^d \) with respect to the vertices \( \{v_i\}_{i=1}^d \) as shown in Figure 1, is the graph obtained from the graphs \( G_1, G_2, \ldots, G_d \) by connecting the vertices \( v_i \) and \( v_{i+1} \) by an edge for all \( i = 1, 2, \ldots, d-1 \).

\textbf{Definition 3.} The bridge graph \( B_2 = B_2(G_1, G_2, \ldots, G_d; v_1, v_2, w_2, v_3, \ldots, v_d, w_d) \) of \( \{G_i\}_{i=1}^d \) with respect to the vertices \( \{v_i, w_i\}_{i=1}^d \) as shown in Figure 2, is the graph obtained from the graphs \( G_1, G_2, G_3, \ldots, G_d \) by connecting the vertices \( w_i \) and \( v_{i+1} \) by an edge for all \( i = 1, 2, \ldots, d-1 \).
Definition 4. The chain graph $C = C(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$ of $\{G_i\}_{i=1}^{d}$ with respect to the vertices $\{v_i, w_i\}_{i=1}^{d}$ as shown in Figure 3, is the graph obtained from the graphs $G_1, G_2, \ldots, G_d$ by identifying the vertices $w_i$ and $v_{i+1}$ for all $i = 1, 2, \ldots, d - 1$.

2. First and third leap Zagreb indices of bridge and chain graphs

2.1. The bridge graph $B_1$

![Figure 1. The bridge graph $B_1$.](image)

The following lemma gives the 2-degree of any arbitrary vertex in the bridge graph $B_1$.

Lemma 5. Let $G_1, G_2, \cdots, G_d$ be $d \geq 5$ connected graphs. Then the 2-degree of any arbitrary vertex $u$ in the bridge graph $B_1$ formed by these graphs is as follows:

$$d_2(u : B_1) = \begin{cases} v_1 + \mu_2 + 1, & \text{if } u = v_1 \\ v_d + \mu_{d-1} + 1, & \text{if } u = v_d \\ v_2 + \mu_1 + \mu_3 + 1, & \text{if } u = v_2 \\ v_{d-1} + \mu_d + \mu_{d-2} + 1, & \text{if } u = v_{d-1} \\ v_i + \mu_{i-1} + \mu_{i+1} + 2, & \text{if } u = v_i, \ 3 \leq i \leq d - 2 \\ d_2(u : G_i) + 1, & \text{if } u \in N_{G_i}(v_1) \\ d_2(u : G_i) + 1, & \text{if } u \in N_{G_i}(v_d) \\ d_2(u : G_i) + 2, & \text{if } u \in N_{G_i}(v_i), \ 2 \leq i \leq d - 1 \\ d_2(u : G_i), & \text{if } u \in V(G_i) \setminus N_{G_i}[v_i], \ 1 \leq i \leq d \end{cases}$$

(2.1)

where $v_i = d_2(v_i : G_i)$ and $\mu_i = \text{deg}(v_i : G_i)$, $1 \leq i \leq d$.

Next, we compute the first leap Zagreb index of the type-I bridge graph $B_1$. Let

$$S_i = \sum_{u \in N_{G_i}(v_i)} d_2(u : G_i), \ 1 \leq i \leq d.$$ 

Theorem 6. $LM_1(B_1) = \sum_{i=1}^{d} LM_i(G_i) + \sum_{i=2}^{d-1} \left( \mu_{i-1} + \mu_{i+1} + 1 \right)^2 + 2v_i(\mu_{i-1} + \mu_{i+1} + 1) + 4S_i + 8\mu_i \right] + 2 \sum_{i=3}^{d-2} \nu_i + 2(S_1 + S_d) + (\mu_1 + \mu_d - 2\mu_3 - 2\mu_{d-2}) + (\mu_2 + 1)(\mu_2 + 2\nu_1 + 1) + (\mu_{d-1} + 1)(\mu_{d-1} + 2\nu_d + 1) + 3d - 12.

Proof. By virtue of Lemma 5

$$LM_1(B_1) = \sum_{u \in V(B_1)} d_2(u : B_1)^2 = (v_1 + \mu_2 + 1)^2 + (v_d + \mu_{d-1} + 1)^2 + (v_2 + \mu_1 + \mu_3 + 1)^2 + (v_{d-1} + \mu_d + \mu_{d-2} + 1)^2$$
Thus the result follows. 

Lemma 8. [1] The degree of an arbitrary vertex $u$ of the bridge graph $B_1$, $d \geq 5$ is given by:

$$deg(u : B_1) = \begin{cases} 
\mu_1 + 1, & \text{if } u = v_1 \\
\mu_d + 1, & \text{if } u = v_d \\
\mu_i + 2, & \text{if } u = v_i, \ 2 \leq i \leq d - 1 \\
\deg(u : G_i), & \text{if } u \in V(G_i) \setminus \{v_i\}, \ 1 \leq i \leq d
\end{cases} \quad (2.2)$$

where $\mu_i = \deg(v_i : G_i)$, $1 \leq i \leq d$.

Next, we compute the third leap Zagreb index of the type-I bridge graph $B_1$. Let us denote $s_i = \sum_{u \in N_G(v_i)} \deg(u : G_i)$, $1 \leq i \leq d$. 

Corollary 7. If $G_1 = G_2 = \cdots = G_d = G$ in a bridge graph $B_1$, then $LM_3(B_1) = dLM_3(G) + (4d - 6)\mu^2 + (4d - 8)v + (12d - 26)\mu + (4d - 4)(\nu\mu + S) + 4d - 12$, where $S = \sum_{u \in N_G(v)} d^2(u : G)$.
Theorem 9. $LM_3(B_1) = \sum_{i=1}^{d} LM_3(G_i) + (s_1 + s_d) + 2 \sum_{i=2}^{d-1} s_i + \sum_{i=1}^{d} (2v_i + 6\mu_i) + 2 \sum_{i=2}^{d} (\mu_{i-1}\mu_i) - 2(\mu_2 + \mu_{d-1}) - (v_1 + v_d) - 3(\mu_1 + \mu_d) + 4d - 10.$

Proof. By virtue of Lemma 5 and 8

\[
LM_3(B_1) = \sum_{u \in \mathbb{B}_1} d_2(u)\deg(u) \\
= (v_1 + \mu_2 + 1)(\mu_1 + 1) + (v_2 + \mu_1 + \mu_3 + 1)(\mu_2 + 2) + (v_d + \mu_{d-1} + 1)(\mu_d + 1) \\
+ (v_{d-1} + \mu_d + \mu_{d-2} + 1)(\mu_{d-1} + 2) + \sum_{i=3}^{d-2} (v_i + \mu_{i-1} + \mu_{i+1} + 2)(\mu_i + 2) \\
+ \sum_{u \in N_{G_1}(v_1)} (d_2(u : G_1) + 1)(\deg(u : G_1)) + \sum_{u \in N_{G_d}(v_d)} (d_2(u : G_d) + 1)(\deg(u : G_d)) \\
+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i)} (d_2(u : G_i) + 2)(\deg(u : G_i)) + \sum_{i=1}^{d} \sum_{u \in V(G_i) \setminus N_{G_i}(v_i)} (d_2(u : G_i))(\deg(u : G_i)) \\

= (v_1\mu_1 + v_1 + \mu_2\mu_1 + \mu_2 + \mu_1 + 1) + (v_2\mu_2 + 2v_2 + \mu_1\mu_2 + 2\mu_1 + \mu_3\mu_2 + 2\mu_3 + \mu_2 + 2) \\
+ (v_d\mu_d + v_d + \mu_{d-1}\mu_d + \mu_{d-1} + \mu_d + 1) + (v_{d-1}\mu_{d-1} + 2v_{d-1} + \mu_d\mu_{d-1}) \\
+ 2\mu_d + \mu_{d-2}\mu_{d-1} + 2\mu_{d-2} + \mu_{d-1} + 2) + \sum_{i=3}^{d-2} (v_i\mu_i + 2v_i + \mu_{i-1}\mu_i + 2\mu_{i-1} + \mu_{i+1}\mu_i) \\
+ 2\mu_{i+1} + 2\mu_i + 4) + \sum_{u \in N_{G_1}(v_1)} (d_2(u : G_1)\deg(u : G_1) + \deg(u : G_1)) + \sum_{u \in N_{G_d}(v_d)} (d_2(u : G_d)\deg(u : G_d) \\
+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i)} (d_2(u : G_i)\deg(u : G_i) + 2\deg(u : G_i)) \\
+ \sum_{i=1}^{d} \sum_{u \in V(G_i) \setminus N_{G_i}(v_i)} d_2(u : G_i)\deg(u : G_i)
\]

Thus the result follows.

Corollary 10. If $G_1 = G_2 = \cdots = G_d = G$ in a bridge graph $B_1$, then $LM_3(B_1) = dLM_3(G) + 2(d - 1)(s + v + \mu^2) + 2\mu(3d - 5) + 4d - 10$, where $s = \sum_{u \in N_G(v)} \deg(u : G)$.

2.2. The bridge graph $B_2$

![Figure 2. The bridge graph $B_2$.](image-url)
Proof.

Theorem 12. LM₁(ℬ₂) = Σ_{i=1}^{d} LM₁(G_i) + 2(S¹ + S₂) + (λ₁ + μ_d) +
Σ_{i=2}^{d-1} Σ_{w ∈ N_{G_i}(v_i) \cup N_{G_i}(w_i)} [2d₂(u : G_i) + 1] + 4 Σ_{i=2}^{d-1} Σ_{u ∈ N_{G_i}(v_i) \cup N_{G_i}(w_i)} [d₂(u : G_i) + 1] + Σ_{i=1}^{d-1} (μ_i^2 + 2δ_iμ_{i+1}) + Σ_{i=2}^{d} (λ_{i-1}^2 + 2v_iλ_{i-1}).

Proof.

LM₁(ℬ₂) = Σ_{u ∈ V(ℬ₂)} d₂(u : ℬ₂)^2
= Σ_{u ∈ V(G_1)} d₂(u : G_1)^2 + Σ_{i=2}^{d} Σ_{u ∈ V(G_i) \cup N_{G_i}(w_i)} d₂(u : G_i)^2
+ Σ_{u ∈ V(G_d) \cup N_{G_d}(w_d)} d₂(u : G_d)^2 + Σ_{u ∈ N_{G_1}(v_1)} (d₂(u : G_1) + 1)^2
+ Σ_{i=2}^{d-1} Σ_{w ∈ N_{G_i}(v_i) \cup N_{G_i}(w_i)} (d₂(u : G_i) + 1)^2
+ Σ_{w ∈ N_{G_d}(v_d)} (d₂(u : G_d) + 1)^2 + Σ_{i=2}^{d-1} Σ_{w ∈ N_{G_i}(v_i) \cup N_{G_i}(w_i)} (d₂(u : G_i) + 2)^2.
Lemma 14.

\[ + \sum_{i=1}^{d-1} (\delta_i + \mu_{i+1})^2 + \sum_{i=2}^{d} (v_i + \lambda_{i-1})^2 \]

\[ = LM_1(G_1) - \delta_1^2 - \sum_{u \in N_G(w_1)} d_2(u : G_1)^2 + \sum_{i=2}^{d-1} \left[ \sum_{u \in V(G_i)} d_2(u : G_i)^2 - \sum_{u \notin V(G_{i+1}) \cup N_{G_i}(w_i)} d_2(u : G_i)^2 + v_i^2 - \delta_i^2 \right] \]

\[ + LM_1(G_d) - v_d^2 - \sum_{u \in N_{G_d}(v_d)} d_2(u : G_d)^2 + \sum_{u \in N_{G_1}(w_1)} d_2(u : G_1) + \lambda_1 + \sum_{i=2}^{d} d_2(u : G_i) + 1 \]

\[ + \sum_{i=2}^{d-1} \left[ \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} [d_2(u : G_i)^2 + 2d_2(u : G_i) + 1] + \sum_{u \in N_{G_d}(v_d)} [d_2(u : G_d)^2 + 2d_2(u : G_d) + 1] \right] \]

\[ + \sum_{i=2}^{d-1} \left[ \sum_{u \in N_{G_i}(v_i) \cap N_{G_i}(w_i)} [d_2(u : G_i)^2 + 4d_2(u : G_i) + 4] \right] \]

\[ + \sum_{i=1}^{d} [\delta_i^2 + 2\delta_i \mu_{i+1} + \mu_{i+1}^2] + \sum_{i=2}^{d} [v_i^2 + 2v_i \lambda_{i-1} + \lambda_{i-1}^2] \]

Thus,

\[ LM_1(B_2) = \sum_{i=1}^{d} LM_1(G_i) + 2(S_1 + S_d) + (\lambda_1 + \mu_d) \]

\[ + \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \setminus N_{G_i}(w_i)} [2d_2(u : G_i) + 1] + 4 \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \cap N_{G_i}(w_i)} [d_2(u : G_i) + 1] \]

\[ + \sum_{i=1}^{d} (\mu_{i+1}^2 + 2\delta_i \mu_{i+1}) + \sum_{i=2}^{d} (\lambda_{i-1}^2 + 2v_i \lambda_{i-1}). \]

\[ \square \]

Corollary 13. If \( G_1 = G_2 = \cdots = G_d = G \), in a bridge graph \( B_2 \), then \( LM_1(B_2) = dLM_1(G) + \lambda + \mu + 2(S + S') + (d-2) \sum_{u \in N_G(v) \setminus N_G(w)} (2d_2(u : G) + 1) + 4(d-2) \sum_{u \in N_G(v) \setminus N_G(w)} (d_2(u : G) + 1) + (d-1)[\mu^2 + \lambda^2] + 2(d-1)[\delta \mu + v \lambda] \), where \( S = \sum_{u \in N_G(v)} d_2(u : G) \) and \( S' = \sum_{u \in N_G(w)} d_2(u : G) \).

In what follows next, we compute the third leap Zagreb index of \( B_2 \).

Lemma 14. The degree of an arbitrary vertex \( u \) of the bridge graph \( B_2, d \geq 5 \) is given by:

\[ \deg(u : B_2) = \begin{cases} 
\deg(u : G_1), & \text{if } u \in V(G_1) \setminus \{w_1\} \\
\deg(u : G_d), & \text{if } u \in V(G_d) \setminus \{v_d\} \\
\deg(u : G_i), & \text{if } u \in V(G_i) \setminus \{v_i, w_i\}, \ 2 \leq i \leq d-1 \\
\lambda_i + 1, & \text{if } u = w_i, \ 1 \leq i \leq d-1 \\
\mu_i + 1, & \text{if } u = v_i, \ 2 \leq i \leq d. \end{cases} \quad (2.4) \]

where \( \mu_i = \deg(v_i : G_i) ; 2 \leq i \leq d, \ \lambda_i = \deg(w_i : G_i) ; 1 \leq i \leq d-1. \)
Theorem 15. \[ LM_3(\mathcal{B}_2) = \sum_{i=1}^{d} LM_3(G_i) + \sum_{u \in N_{G_1}(v_1)} \deg(u : G_1) + \sum_{u \in N_{G_d}(v_d)} \deg(u : G_d) \]
\[ + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_{i-1}}(v_{i-1})} \deg(u : G_i) \]
\[ + \sum_{i=1}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_{i+1}}(v_{i+1})} \deg(u : G_{i+1}) \]
\[ + \sum_{i=1}^{d-1} \sum_{u \in N_{G_{i+1}}(v_{i+1}) \setminus N_{G_i}(v_i)} \deg(u : G_i) + 2 \deg(u : G_1) \]
\[ + \sum_{i=1}^{d-1} (\delta_i + \mu_{i+1})(\lambda_i + 1) + \sum_{i=2}^{d} (v_i + \lambda_{i-1})(\mu_i + 1) + \delta \delta_d. \]

Proof. By virtue of Lemma 11 and 14
\[ LM_3(\mathcal{B}_2) = \sum_{u \in V(\mathcal{B}_2)} d_2(u) \deg(u) \]
\[ = \sum_{u \in V(G_1) \setminus N_{G_1}(v_1)} d_2(u : G_1) \deg(u : G_1) + \sum_{i=2}^{d-1} \sum_{u \in V(G_i) \setminus (N_{G_i}(v_i) \cup N_{G_{i-1}}(v_{i-1}))} d_2(u : G_i) \deg(u : G_i) \]
\[ + \sum_{u \in V(G_d) \setminus N_{G_d}(v_d)} d_2(u : G_d) \deg(u : G_d) + \sum_{i=2}^{d-1} (d_2(u : G_i) + 1)(\deg(u : G_1)) \]
\[ + \sum_{i=1}^{d-1} (d_2(u : G_i) + 1)(\deg(u : G_i)) + \sum_{i=2}^{d-1} \sum_{u \in V(G_i) \setminus N_{G_i}(v_i)} \deg(u : G_i) \]
\[ + \sum_{i=1}^{d-1} (d_2(u : G_i) + 2)(\deg(u : G_i)) + \sum_{i=1}^{d-1} (\delta_i + \mu_{i+1})(\lambda_i + 1) + \sum_{i=2}^{d} (v_i + \lambda_{i-1})(\mu_i + 1) + \delta \delta_d. \]

Thus the result follows. \[\square\]

Corollary 16. If \( G_1 = G_2 = \cdots = G_d = G \) in a bridge graph \( \mathcal{B}_2 \), then
\[ LM(\mathcal{B}_2) = dLM(G) + \sum_{u \in N_G(v)} \deg(u : G) + \sum_{u \in N_G(v)} \deg(u : G) + (d-2)(\sum_{u \in N_G(v) \setminus N_{G(u)}} \deg(u : G)) \]
\[ + \sum_{u \in N_G(v) \setminus N_{G(u)}} 2 \deg(u : G)) + (d-1)(2\mu \lambda + \mu + \lambda) + d(\delta + \nu) - (\nu + \delta). \]

2.3. The chain graph \( C \)

In the following lemma, we obtain the 2-degree of any vertex in the chain graph \( C \).

Lemma 17. Let \( G_1, G_2, \ldots, G_d, d \geq 5 \) be \( C_3 \)-free connected graphs and let \( \mathcal{C} = C(G_1, G_2, \ldots, G_d; v_1, v_2, v_3, \ldots, v_{d-1}, v_d) \) be the chain graph formed using these graphs. Then the 2-degree of any vertex \( u \) in \( C \) is given as follows:

\[ \ldots \]
\[ \text{Proof.} \]

Theorem 18. For the chain graph \( C \),

\[
\begin{align*}
LM_1(C) &= \sum_{i=1}^{d} LM_i(G_i) + \sum_{u \in N_{G_i}(w_i)} [2\mu_2 d_2(u : G_1) + \mu_2^2] + \sum_{u \in N_{G_i}(v_d)} [2\lambda_{d-1} d_2(u : G_d) + \lambda_{d-1}^2] \\
&+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(w_i)} [2\mu_{i+1} d_2(u : G_i) + \mu_{i+1}^2] + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i)} [2\lambda_{i-1} d_2(u : G_i) + \lambda_{i-1}^2] \\
&+ 2 \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(w_i) \cap N_{G_i}(v_i)} [\lambda_{i-1} d_2(u : G_i) + \mu_{i+1} d_2(u : G_i) + \lambda_{i-1} \mu_{i+1}] \\
&+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \cap N_{G_i}(w_i)} (\lambda_{i-1}^2 + \mu_{i+1}^2) + 2 \sum_{i=1}^{d-1} \delta_i \nu_i + 1.
\end{align*}
\]

Proof. By Lemma 17, we have

\[
LM_1(C) = \sum_{u \in V(C)} d_2(u : C)^2 = \sum_{u \in V(G_1)} d_2(u : G_1)^2 + \sum_{u \in N_{G_1}(w_1)} [d_2(u : G_1) + \mu_2]^2 + \sum_{u \in V(G_d) \setminus N_{G_d}(v_d)} d_2(u : G_d)^2 + \sum_{u \in N_{G_d}(v_d)} [d_2(u : G_d) + \lambda_{d-1}]^2 + \sum_{i=2}^{d-1} \sum_{u \in V(G_i) \setminus (N_{G_i}(v_i) \cup N_{G_i}(w_i))} d_2(u : G_i)^2 + \sum_{u \in N_{G_i}(w_i) \cap N_{G_i}(v_i)} [d_2(u : G_i) + \mu_{i+1}]^2 + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} [d_2(u : G_i) + \lambda_{i-1}]^2 + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} [d_2(u : G_i) + \lambda_{i-1} + \mu_{i+1}]^2 + \sum_{i=1}^{d-1} \delta_i \nu_i + 1.
\]
Corollary 19. In a chain graph $C$, if $G_1 = G_2 = \cdots = G_d = G$, then
\[
LM_1(C) = dLM_1(G) + \sum_{u \in V(G)} [2\mu d_2(u : G) + \mu^2] + \sum_{u \in V(G)} [2\lambda d_2(u : G) + \lambda^2] + (d - 2) \sum_{u \in V(G)} [2\mu d_2(u : G) + \mu^2] + (d - 2) \sum_{u \in V(G)} [2\lambda d_2(u : G) + \lambda^2] + 2(d - 2) (\lambda^2 + \mu^2) + 2(\lambda - 2)\delta v.
\]

Lemma 20. Let $G_1, G_2, \ldots, G_d, d \geq 5$ be $C_3$-free connected graphs and let $C = C(G_1, G_2, \ldots, G_d; w_1, v_2, w_2, v_3, \ldots, w_{d-1}, v_d)$ be the chain graph formed using these graphs.
Then the degree of any vertex $u$ in $C$ is given as follows:

$$
\text{deg}(u : C) = \begin{cases} 
\text{deg}(u : G_1), & \text{if } u \in V(G_1) \setminus \{w_1\} \\
\text{deg}(u : G_d), & \text{if } u \in V(G_d) \setminus \{v_d\} \\
\text{deg}(u : G_i), & \text{if } u \in V(G_i) \setminus \{v_i, w_i\}, \quad 2 \leq i \leq d - 1 \\
\lambda_i + \mu_{i+1}, & \text{if } u = w_i = v_{i+1}, \quad 1 \leq i \leq d - 1,
\end{cases}
$$

(2.6)

where $\mu_i = \text{deg}(v_i : G_i)$, $\lambda_i = \text{deg}(w_i : G_i)$ for all $1 \leq i \leq d$

Finally, we compute the third leap Zagreb index of the chain graph $C$ by applying Lemma 17 and 20.

**Theorem 21.** $LM_3(C) = \sum_{i=1}^{d} LM_3(G_i) + \sum_{u \in N_{G_i}(w_1)} \mu_2\text{deg}(u : G_1) + \sum_{u \in N_{G_i}(v_2)} \lambda_{d-1}\text{deg}(u : G_i) + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} \mu_{i+1}\text{deg}(u : G_i) + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} \lambda_{i-1}\text{deg}(u : G_i) + \sum_{i=1}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} \lambda_i\text{deg}(u : G_i) + \sum_{i=1}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} \mu_i\text{deg}(u : G_i) + \sum_{i=1}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} \lambda_{i-1}\text{deg}(u : G_i) + \sum_{i=1}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} \mu_i\text{deg}(u : G_i).

Proof.** By virtue of Lemma 17 and 20

$$
LM_3(C) = \sum_{u \in V(C)} d_2(u)\text{deg}(u)
= \sum_{u \in V(G_1) \setminus N_{G_1}(w_1)} d_2(u : G_1)\text{deg}(u : G_1) + \sum_{u \in N_{G_1}(v_2)} (d_2(u : G_1) + \mu_2)\text{deg}(u : G_1)
+ \sum_{u \in V(G_d) \setminus N_{G_d}(v_d)} d_2(u : G_d)\text{deg}(u : G_d) + \sum_{u \in N_{G_d}(v_d)} (d_2(u : G_d) + \lambda_{d-1})\text{deg}(u : G_d)
+ \sum_{i=2}^{d-1} \sum_{u \in V(G_i) \setminus (N_{G_i}(w_i) \cup N_{G_i}(v_i))} d_2(u : G_i)\text{deg}(u : G_i) + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} (d_2(u : G_i) + \lambda_{i-1})\text{deg}(u : G_i)
+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} (d_2(u : G_i) + \lambda_{i-1} + \mu_{i+1})\text{deg}(u : G_i)
+ \sum_{i=1}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(v_{i+1})} \delta_i + v_{i+1})(\lambda_i + \mu_{i+1}).
$$

Thus the result follows. \[\square\]

**Corollary 22.** In a chain graph $C$, if $G_1 = G_2 = \cdots = G_d = G$, then

$$
LM_3(C) = dLM_3(G) + \sum_{u \in N_{G}(w)} \mu\text{deg}(u : G) + \sum_{u \in N_{G}(v)} \lambda\text{deg}(u : G) + (d - 2)(\sum_{u \in N_{G}(w) \setminus N_{G}(v)} \mu\text{deg}(u : G) + \sum_{u \in N_{G}(v) \setminus N_{G}(w)} \lambda\text{deg}(u : G) + (d - 1)(\delta\mu + \nu\lambda)).
$$

3. Examples

In this section, we determine the first and third leap Zagreb indices of some molecular graph structures.

![Figure 4](image)

**Figure 4.** Ortho, meta and para positions of two vertices in a hexagon $H$.

Two vertices $v$ and $w$ of a hexagon $H (C_6)$ (please refer Figure 4) are said to be in

(i) ortho-position, if they are adjacent in $H$

(ii) meta-position, if they are distance two in $H$

(iii) para-position, if they are distance three in $H$.

We connect $h \geq 5$ ortho-hexagons to form a polyphenyl chain denoted by $O_h$ as follows:

![Figure 5](image)

**Figure 5.** Polyphenyl chain $O_h$.

One can observe that the Polyphenyl chain $O_h$ shown in Figure 5 is a $B_1$ type bridge graph. Therefore, from Corollary 7, we get

\[
LM_1(O_h) = hLM_1(G) + (4h - 6)\mu^2 + (4h - 8)\nu + (12h - 26)\mu + (4h - 4)\nu\mu + \sum_{u \in N_G(v)} d_2(u : G)] + 4h - 12
\]

\[
= 24h + (4h - 6)(4) + (4h - 8)(2) + (12h - 26)(2) + (4h - 4)(4) + (4h - 4)(4) + 4h - 12
\]

\[
= 108h - 136.
\]

Similarly,

From Corollary 10, we get

\[
LM_3(O_h) = 24h + (2h - 2)(2) + (2h - 2)(2) + 2(2)(3h - 5) + 2(h - 1)(2 + 4) + 4h - 10
\]

\[
= 60h - 50
\]
The polyphenyl chain \( M_h \) is formed by connecting \( h \geq 5 \) meta-hexagons as shown in Figure 6.

The polyphenyl chain \( P_h \) is formed by connecting \( h \geq 5 \) para-hexagons as shown in the following Figure 7.

It is clear that the Polyphenyl chains \( M_h \) and \( P_h \) are type-II bridge graphs \( B_2 \).

Using Corollary 13, we get

\[
LM_1(M_h) = hLM_1(G) + \lambda + \mu + 2 \sum_{u \in N_G(w)} d_2(u : G) + (h - 2) \left[ \sum_{u \in N_G(v) \cap N_G(w)} (2d_2(u : G) + 1) \right]
\]

\[
+ (h - 2) \sum_{u \in N_G(v) \cap N_G(w)} (2d_2(u : G) + 1) + 4(h - 2) \sum_{u \in N_G(v) \cap N_G(w)} (d_2(u : G) + 1)
\]

\[
+ 2 \sum_{u \in N_G(v)} d_2(u : G) + (h - 1)\mu^2 + 2(h - 1)\delta \mu + 2(h - 1)\nu \lambda + (h - 1)\lambda^2
\]

\[
= 24h + 4 + 2(4) + (h - 2)(2)(2 + 1) + (h - 2)(2)(2 + 1) + 4(h - 2)(2 + 1) + 2(4) + (h - 1)(4)
\]

\[
+ 4(h - 1)(4) + (h - 1)(4)
\]

Thus \( LM_1(M_h) = 70h - 48 \).

Similarly, by Corollary 13, we have

\[
LM_1(P_h) = 24h + 4 + 2(4) + (h - 2)(2)(2 + 2) + (h - 2)(2)(2 + 1) + 4(h - 2)(2 + 1) + 2(4) + (h - 1)(4)
\]

\[
+ 8(h - 1) + 8(h - 1) + (h - 1)(4)
\]

Therefore, \( LM_1(P_h) = 68h - 44 \).

Using Corollary 16, we get

\[
LM_3(M_h) = 24h + 8 + (h - 2)8 + (h - 1)12 + h(4) - 4
\]
= 48h − 24

\[ LM_3(P_h) = 24h + 8 + (h − 2)8 + (h − 1)12 + 4h − 4 \]
= 48h − 24.

Next, we shall see an application related to the chain graph \( C \). The spiro-chain \( SPC_4(d, 3) \) is a chain graph formed using \( d \geq 5 \) copies of the cycle \( C_4 \).
Here the number 3 in the construction denotes the position of the vertices \( v \) and \( w \) in the spiro-chain (refer Figure 8).

![Figure 8](image)

**Figure 8.** Spiro-chain \( SPC_4(d, 3) \) formed with \( d \geq 5 \) copies of \( C_4 \) connected in 3rd position.

The spiro-chain \( SPC_6(d, 4) \) is a chain graph formed using \( d \geq 5 \) copies of the cycle \( C_6 \) or hexagon where the vertices \( v \) and \( w \) are connected in the 4th position (refer Figure 9).

![Figure 9](image)

**Figure 9.** Spiro-chain \( SPC_6(d, 4) \) formed with \( d \geq 5 \) copies of \( C_6 \) connected in 4th position.

By applying Corollary 19, we get

\[ LM_1(SPC_4(d, 3)) = dLM_1(G) + \sum_{u \in N_G(v)} [2\mu d_2(u : G) + \mu^2] + \sum_{u \in N_G(w)} [2\lambda d_2(u : G) + \lambda^2] \]
\[ + (d − 2) \sum_{u \in N_G(v) \cap N_G(w)} [\lambda d_2(u : G) + \mu d_2(u : G) + \lambda \mu] \]
\[ + 2(d − 2) \sum_{u \in N_G(v) \cap N_G(w)} (\lambda^2 + \mu^2) + 2(d − 1)\delta v \]
\[ = 54d − 66. \]

Similarly, from Corollary 19, we have \( LM_1(SPC_6(d, 4)) = 80d − 56. \)

By applying Corollary 22, we get

\[ LM_3(SPC_4(d, 3)) = 8d + 2(2 + 2) + 2(2 + 2) + (d − 2)(16) + (d − 1)(4) \]
\[ = 28d − 20 \]

Similarly, from Corollary 22, we have \( LM_3(SPC_6(d, 4)) = 48d − 24. \)
4. Conclusions

We have computed exact values of one of the recent topological invariants namely first and third leap Zagreb indices for bridge and chain graphs. It is worth mentioning that computing second leap Zagreb index of bridges and chain graphs has not yet addressed and interested researchers may work on it. Also these indices need to be explored for several other interesting graph structures arising from mathematical chemistry and other branches of science.

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Conflict of interest

The authors declare that no competing interests exist.

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